Can entanglement hide behind triangle-free graphs?*

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(Dated: October 28, 2020)

We present a novel approach to unveil a new kind of entanglement in bipartite quantum states with "triangle-free" zero-patterns on their diagonals. Upon application of a local averaging operation, the separability of such states transforms into a simple positivity condition, violation of which implies the presence of entanglement. Using this strategy, we develop a recipe to construct unique classes of PPT entangled triangle-free states in arbitrary dimensions. Finally, we link the task of entanglement detection in general states to the problem of finding triangle-free induced subgraphs in a given graph.

arXiv:2010.11891v2 [quant-ph] 27 Oct 2020

I. INTRODUCTION

Termed "spooky action at a distance" by Einstein, quantum entanglement has come a long way since its inception in the first half of the 20^{th} century [1, 2] — both in terms of theoretical and experimental relevance. Now understood as one of the most fundamental non-classical features of quantum theory, entanglement has garnered a reputation as a resource of immense practical worth, with its groundbreaking effects visible in a wide array of quantum cryptographic [3, 4], teleportation [5] and computation [6] protocols. However, even after more than 85 years of its discovery, the theory of entanglement has managed to retain its richness and complexity.

First concrete signs of entanglement were explored by Bell in terms of violations of spin correlation inequalities [7], which were later shown by Werner to be sufficient but not necessary to detect entanglement [8]. Connections with the theory of positive maps were not made until the late '90s, when positivity under partial transposition (PPT) was shown by Peres to be a necessary condition for separability [9], which was later also proved to be sufficient in low dimensional $2 \otimes 2$ and $2 \otimes 3$ systems [10]. Since then, the study of separability has witnessed tremendous growth, with a myriad of tests now available to detect entanglement in various different scenarios, see [11, Section VI B] and [12]. The primary goal of all these tests is to bypass a major theoretical hurdle which is intrinsic to the structure of entanglement itself, namely, the NP-hardness of the weak membership problem for the convex set of separable bipartite states [13]. Put simply, it is not possible for any classical algorithm to efficiently determine whether a given state is entangled or not (assuming that the widely believed P$\neq$NP result holds). Still, several algorithms with complexities scaling exponentially with the system dimension do exist [14–16].

In this letter, we unearth a new kind of entanglement in bipartite states, which is easy to detect but rich enough to manifest itself in astonishing variety. For a $d \otimes d$ state, this entanglement camouflages beneath an intriguing design of zeros on the state's diagonal, which, when rearranged in the form of a $d \times d$ matrix, reveals a distinctive "triangle-free" (Δ-free) zero-pattern in the off-diagonal part of the matrix. The terminology is akin to the one used in graph theory, where Δ-free graphs have been a subject of interest for well over a century. To detect entanglement in these Δ-free states, we project them onto the subspace of local diagonal orthogonal invariant (LDOI) matrices, through a local operation which preserves the separability and Δ-free property of states. LDOI states have been amply scrutinized in literature, [17–20], since many important examples of PPT (and NPT) states are of this type: Werner and Isotropic states [8, 21], Diagonal Symmetric states [22, 23], canonical NPT states [24], to name a few (see also [20, Section 3]). Separable states in this class admit an equivalent description in terms of the cone of triplewise completely positive matrices, which is a generalization of the well-studied cone of completely positive matrices [25]. The already established significance of Δ-free graphs within the theory of completely positive matrices [25, Section 2.4] is the primary source of inspiration for the results we present here. We will see that separability in Δ-free LDOI states materializes into simple positivity conditions on certain associated matrices, enabling one to easily detect entanglement in such states. As the number of Δ-free zero patterns increases rather tremendously with the system's dimensions, so does the number of distinct Δ-free entangled families of states. For perspective, in a $15 \otimes 15$ system, we'll provide an explicit way to construct $\sim 10^{10}$ distinct families of PPT entangled Δ-free states. Because of this sheer diversity, the traditional methods for entanglement detection get crippled in the regime of Δ-free states. In contrast, the simplicity of our method cannot be overstated, which provides a highly non-trivial yet computationally efficient technique for entanglement detection in a wide array of scenarios.

Let us now briefly comment on this letter's organization. In Section II, we review the theory of LDOI states and graphs. Section III contains the primary entanglement test and hence forms the core of this letter. A systematic scheme to construct new families of PPT entangled Δ-free states is articulated in Section IV. Section V discusses entanglement detection in non Δ-free states, and connects it to the triangle-free induced subgraph problem. Finally, Section VI presents a summary of our results and important directions for future work.

* Spoiler alert: Yes, it can!
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II. PRELIMINARIES

A. Local diagonal orthogonal invariant states

We will exclusively be dealing with the finite d-dimensional complex Hilbert space $\mathbb{C}^d$ and the space of $d \times d$ complex matrices $\mathcal{M}_d$, with the canonical bases $\{|i\rangle\}_{i=1}^d$ and $\{|i\rangle\langle j|\}_{i,j=1}^d$, respectively. *Positive semi-definite* and *entrywise non-negative* matrices in $\mathcal{M}_d$ will be denoted by $A \geq 0$ and $A \succcurlyeq 0$ respectively. *Quantum states* ($A \geq 0$, $\operatorname{Tr} A = 1$) will be denoted by ρ. We define $[d] \coloneqq \{1, 2, \ldots, d\}$. The following class of bipartite states in $\mathcal{M}_d \otimes \mathcal{M}_d$ will play a crucial role in this letter:

$$\rho_{A,B,C} = \sum_{i,j=1}^{d} A_{ij} |ij\rangle\langle ij| + \sum_{1\leq i\neq j\leq d} B_{ij} |ii\rangle\langle jj| + \sum_{1\leq i\neq j\leq d} C_{ij} |ij\rangle\langle ji| \quad (1)$$

where $A, B, C \in \mathcal{M}_d$ are matrices such that $\operatorname{diag} A = \operatorname{diag} B = \operatorname{diag} C$, $A \succcurlyeq 0$, $B \geq 0$, $C = C^\dagger$, $A_{ij}A_{ji} \geq |C_{ij}|^2$ $\forall i, j \in [d]$ and $\sum_{ij} A_{ij} = 1$. These conditions ensure that $\rho_{A,B,C}$ is indeed a quantum state, as can easily be checked. If the partial transpose $\rho^\Gamma_{A,B,C} \geq 0$ as well (i.e. ρ is PPT), then $C \geq 0$ and $A_{ij}A_{ji} \geq |B_{ij}|^2$ $\forall i, j \in [d]$ [20, Lemma 2.12, 2.13]. These states enjoy a special *local diagonal orthogonal invariance* (LDOI) property:

$$\forall O \in \mathcal{DO}_d, \quad \rho_{A,B,C} = (O \otimes O)\rho_{A,B,C}(O \otimes O) \quad (2)$$

where the group of *diagonal orthogonal* matrices in $\mathcal{M}_d$ is denoted by $\mathcal{DO}_d$. For an arbitrary state $\rho \in \mathcal{M}_d \otimes \mathcal{M}_d$, we define matrices $A, B, C \in \mathcal{M}_d$ entrywise as $A_{ij} = \langle ij|\rho|ij\rangle$, $B_{ij} = \langle ii|\rho|jj\rangle$, and $C_{ij} = \langle ij|\rho|ji\rangle$ for $i, j \in [d]$. Then, the local averaging operation in Eq. (3) acts as the orthogonal projection onto the subspace of LDOI matrices, where O is a random diagonal orthogonal matrix with uniformly random signs $\{\pm\}$ on its diagonal, which are independent and identically distributed (i.i.d):

$$\rho \mapsto \mathbb{E}_O[(O \otimes O)\rho(O \otimes O)] = \rho_{A,B,C} \quad (3)$$

Now, if C is diagonal in Eq. (1), we obtain an important subclass of LDOI states, which is defined by the *conjugate local diagonal unitary invariance* (CLDUI) property:

$$\rho_{A,B} = \sum_{i,j=1}^{d} A_{ij} |ij\rangle\langle ij| + \sum_{1\leq i\neq j\leq d} B_{ij} |ii\rangle\langle jj| \quad (4)$$

$$\forall U \in \mathcal{DU}_d, \quad \rho_{A,B} = (U \otimes U^\dagger)\rho_{A,B}(U^\dagger \otimes U) \quad (5)$$

where $\mathcal{DU}_d$ is the group of *diagonal unitary* matrices in $\mathcal{M}_d$. Analogous to Eq. (3), the local averaging operation in Eq. (6) defines the orthogonal projection onto the subspace of CLDUI matrices, where U is a random diagonal unitary matrix having uniform, i.i.d entries on the unit circle in $\mathbb{C}$ and $A, B \in \mathcal{M}_d$ are as defined before.

$$\rho \mapsto \mathbb{E}_U[(U \otimes U^\dagger)\rho(U^\dagger \otimes U)] = \rho_{A,B} \quad (6)$$

Remark II.1. *If B is diagonal in Eq. (1), we get the subclass of* local diagonal unitary invariant (LDUI) *states, which we choose not to deal with in this letter. Since the two classes are linked through the operation of partial transposition, the separability results for* CLDUI *states will identically apply to* LDUI *states as well.*

We now define the notions of *pairwise* and *triplewise completely positive* (PCP and TCP) matrices, which are fundamentally connected to the separability of the CLDUI and LDOI states, respectively. For $|v\rangle, |w\rangle \in \mathbb{C}^d$, we denote the operations of entrywise complex conjugate and Hadamard product in $\mathbb{C}^d$ by $|\bar{v}\rangle$ and $|v \odot w\rangle$, respectively. Recall that $\rho \in \mathcal{M}_d \otimes \mathcal{M}_d$ (un-normalized) is said to be *separable* if there exist a finite set of vectors $\{|v_k\rangle, |w_k\rangle\}_{k\in I} \subset \mathbb{C}^d$ such that $\rho = \sum_{k\in I} |v_k w_k\rangle\langle v_k w_k|$.

Theorem II.2. *Let $A, B, C \in \mathcal{M}_d$. Then,*

- $\rho_{A,B}$ *is separable* $\iff$ (A, B) *is* PCP $\iff$ *there exist vectors* $\{|v_k\rangle, |w_k\rangle\}_{k\in I} \subset \mathbb{C}^d$ *such that*

$$A = \sum_{k\in I} |v_k \odot \overline{v_k}\rangle\langle w_k \odot \overline{w_k}| \quad B = \sum_{k\in I} |v_k \odot w_k\rangle\langle v_k \odot w_k|$$

- $\rho_{A,B,C}$ *is separable* $\iff$ (A, B, C) *is* TCP $\iff$ *there exist vectors* $\{|v_k\rangle, |w_k\rangle\}_{k\in I} \subset \mathbb{C}^d$ *such that*

$$A = \sum_{k\in I} |v_k \odot \overline{v_k}\rangle\langle w_k \odot \overline{w_k}| \quad B = \sum_{k\in I} |v_k \odot w_k\rangle\langle v_k \odot w_k|$$

$$C = \sum_{k\in I} |v_k \odot \overline{w_k}\rangle\langle v_k \odot \overline{w_k}|$$

Proof. See [18, Theorem 5.2] or [20, Theorem 2.9]. □

B. Graphs

A (simple, undirected) *graph* G consists of a finite *vertex* set V, together with a finite set of two-element (unordered) subsets of V, known as the *edge* set E. G can be represented pictorially by drawing the elements (vertices) of V as points, with $i, j \in V$ connected by a line if $\{i, j\} \in E$. For two graphs $G = (V_G, E_G)$ and $H = (V_H, E_H)$, we say that G *contains* H ($H \subseteq G$) if $V_H \subseteq V_G$ and $E_H \subseteq E_G$. An l-cycle (denoted C_l) in a graph is a sequence of edges $\{i_0, i_1\}, \{i_1, i_2\}, \ldots, \{i_{l-1}, i_l\}$ such that $i_1 \neq i_2 \neq \ldots \neq i_l$, and $i_0 = i_l$. 3-cycles are called triangles. A graph which does not contain any triangles is called Δ-*free*. A graph is termed *cyclic* if it contains a cycle and *acyclic* otherwise. Given a matrix $A \in \mathcal{M}_d$, we associate a graph $G(A)$ to it on d vertices such that for $i \neq j$, $\{i, j\}$ is an edge if both A_{ij} and A_{ji} are non-zero. The *adjacency matrix* $A \in \mathcal{M}_d$ of a graph G (denoted $\operatorname{ad} G$) on d vertices is defined as follows: $\operatorname{diag} A = 0$ and $A_{ij} = A_{ji} = 1$ if $\{i, j\}$ is an edge for $i \neq j$. If G is a graph on d vertices, then $B \in \mathcal{M}_d$ is called a matrix realization of G if $G(B) = G$. We refer the readers to the excellent book by Bondy and Murty [26] for a more thorough introduction to graphs.

III. MAIN RESULTS

Maintaining close proximity with the graph-theoretic terminology, we begin by introducing the concept of *triangle-free* (Δ*-free*) bipartite states.

Definition III.1. *A bipartite state $\rho \in \mathcal{M}_d \otimes \mathcal{M}_d$ is said to be* triangle-free *(Δ-free) if the associated matrix $A \in \mathcal{M}_d$ defined entrywise as $A_{ij} = \langle ij|\rho|ij\rangle$ for $i, j \in [d]$, is such that $G(A)$ is Δ-free.*

From the definition, it is clear that the property of Δ-freeness of a state is nothing but a statement on the zero pattern of the state's diagonal. It is not too difficult to ascertain whether a state has this property, as efficient polynomial-time algorithms exist to determine whether a graph G is Δ-free [27]; for example, $\operatorname{trace}[(\operatorname{ad} G)^3] = 0 \iff G$ is Δ-free. We now proceed towards exploiting the Δ-free property of an LDOI state to obtain a powerful necessary condition for its separability. Recall that for a vector $|v\rangle \in \mathbb{C}^d$, $\operatorname{supp}|v\rangle := \{i \in [d] : \langle i|v\rangle \neq 0\}$. We define $\sigma(v)$ to be the size of $\operatorname{supp}|v\rangle$. For $B \in \mathcal{M}_d$, the comparison matrix $M(B)$ is defined as $M(B)_{ij} = |B_{ij}|$ for $i = j$ and $M(B)_{ij} = -|B_{ij}|$ otherwise. It is crucial to note that for $B \geq 0$, $M(B)$ need not be positive semi-definite. In fact, the constraint $M(B) \geq 0$ is far from trivial and is actually used to define the so called class of H-matrices [28, Chapter 6]. However, it turns out that the Δ-freeness of $\rho_{A,B,C}$ is strong enough to ensure that above constraint holds for $B, C \geq 0$, as we now show.

Theorem III.2. *If $\rho_{A,B,C}$ is Δ-free and separable, then $M(B)$ and $M(C)$ are positive semi-definite.*

Proof. Since $\rho_{A,B,C}$ is separable, (A, B, C) is TCP and there exist vectors $\{|v_k\rangle, |w_k\rangle\}_{k\in I} \subset \mathbb{C}^d$ such that the decomposition in Theorem II.2 holds. Now, if there exists a $k \in I$ such that $\sigma(v_k \odot w_k) \geq 3$, then $G(|v_k \odot \overline{v_k}\rangle\langle w_k \odot \overline{w_k}|)$ (and hence $G(A)$) would contain a triangle, which is not possible since $\rho_{A,B,C}$ is Δ-free. Hence, $\sigma(v_k \odot w_k) = \sigma(v_k \odot \overline{w_k}) \leq 2$ for each k. Now, let

$$I_1 = \{k \in I : \sigma(v_k \odot w_k) \leq 1\}$$
$$I_{ij} = \{k \in I : \operatorname{supp}|v_k \odot w_k\rangle = \{i, j\}\} \quad (\text{for } i < j)$$

so that the index set splits as $I = I_1 \cup_{i<j} I_{ij}$. Further, if we define $B^{ij} = \sum_{k\in I_{ij}} |v_k \odot w_k\rangle\langle v_k \odot w_k|$, it is easy to see that $M(B^{ij}) \geq 0$ for all $i < j$, since each B^{ij} is supported on a 2-dimensional subspace $\mathbb{C}|i\rangle \oplus \mathbb{C}|j\rangle \subset \mathbb{C}^d$. The following decomposition then shows that $M(B) \geq 0$:

$$M(B) = \sum_{k\in I_1} |v_k \odot w_k\rangle\langle v_k \odot w_k| + \sum_{1\leq i<j\leq d} M(B^{ij})$$

A similar argument shows that $M(C) \geq 0$ as well. ☐

Observe how the Δ-freeness of $G(A)$ above is used to force the vectors v_k, w_k to have small common supports. If we define $A_k = |v_k \odot \overline{v_k}\rangle\langle w_k \odot \overline{w_k}|$ and B_k, C_k as the rank-one projections onto $|v_k \odot w_k\rangle, |v_k \odot \overline{w_k}\rangle$, it is clear that $\rho_{A,B,C} = \sum_k \rho_{A_k,B_k,C_k}$, where the small common supports imply that each ρ_{A_k,B_k,C_k} has support on a $2\otimes 2$ subsystem (barring some diagonal entries). This is what ensures that $M(B), M(C) \geq 0$, as was shown in the proof above. Remarkably, for CLDUI states, the converse also holds (i.e. if $\rho_{A,B}$ is PPT and $M(B) \geq 0$, then $\rho_{A,B}$ is separable). [18, Corollary 5.5]. Hence, we obtain a complete characterization of separable Δ-free CLDUI states.

Theorem III.3. *If $\rho_{A,B}$ is Δ-free and PPT, then $\rho_{A,B}$ is separable $\iff M(B) \geq 0$.*

For LDOI states, the converse of Theorem III.2 ceases to hold, see [20, Example 9.2]. Nevertheless, we do have a non-trivial necessary condition for separability, which we now exploit to arrive at our primary entanglement detection strategy in arbitrary Δ-free states.

Theorem III.4. *Let $\rho \in \mathcal{M}_d \otimes \mathcal{M}_d$ be an arbitrary Δ-free state with the associated matrices $A, B, C \in \mathcal{M}_d$ defined entrywise as $A_{ij} = \langle ij|\rho|ij\rangle$, $B_{ij} = \langle ii|\rho|jj\rangle$, and $C_{ij} = \langle ij|\rho|ji\rangle$ for $i, j \in [d]$. Then, ρ is entangled if either $M(B)$ or $M(C)$ is not positive semi-definite.*

Proof. For LDOI states, the conclusion follows from Theorem III.2. For an arbitrary $\rho \in \mathcal{M}_d \otimes \mathcal{M}_d$, the result follows from the fact that it can be transformed into a Δ-free LDOI state through a separability preserving local operation: $\rho_{A,B,C} = \mathbb{E}_O[(O \otimes O)\rho(O \otimes O)]$. ☐

We should emphasise here that the above test is very easy to implement in practice. After checking whether the state under consideration is Δ-free, one simply needs to extract the appropriate entries from ρ to form the B, C matrices and check for the positivity of the corresponding comparison matrices. The test can also be generalized to work for states $\rho \in \mathcal{M}_{d_1} \otimes \mathcal{M}_{d_2}$ with $d_1 < d_2$, as we now illustrate. First define a $d_1 \times d_2$ matrix (as before) $A_{ij} = \langle ij|\rho|ij\rangle$, with $i \in [d_1]$, $j \in [d_2]$. Now, corresponding to all possible ways of choosing d_1 different columns of A, construct a total of $\binom{d_2}{d_1}$ matrices $\widetilde{A} \in \mathcal{M}_{d_1}$. For each $\widetilde{A}$ with a Δ-free $G(\widetilde{A})$, construct the projector $P = \sum_i |i\rangle\langle i|$, where the sum is over those $i \in [d_2]$ which were chosen to form columns of $\widetilde{A}$. Project the original state ρ locally to obtain a $d_1 \otimes d_1$ Δ-free state $\widetilde{\rho} = (I \otimes P)\rho(I \otimes P)$, and apply the test from Theorem III.4.

Our next result highlights the unsuitability of a certain subset of Δ-free graphs from the perspective of the above test (see Appendix A for a proof).

Proposition III.5. *If $B \geq 0$ is a matrix realization of an acyclic graph, then $M(B) \geq 0$.*

If $\rho_{A,B,C}$ is a PPT LDOI state with acyclic $G(A)$ (which implies that $G(B), G(C)$ are acyclic as well), the above proposition implies that $M(B), M(C) \geq 0$, thus rendering Theorem III.4 incapable of detecting any entanglement. For CLDUI states, Theorem III.3 allows us to trivially prove the following result.

Corollary III.6. *If $\rho_{A,B}$ is such that $G(A)$ is acyclic, then $\rho_{A,B}$ is separable $\iff \rho_{A,B}$ is PPT.*

IV. CONSTRUCTION OF NEW PPT ENTANGLED GRAPH STATES

In Proposition III.5, we saw that Δ-free acyclic graphs forbid the possibility of a matrix realization $B \geq 0$ such that $M(B) \not\geq 0$. We now examine the remaining class of Δ-free graphs which contain a cycle (of length ≥ 4) and show that such graphs do allow for the proposed matrix realizations to exist. (Proof is included in Appendix A).

Proposition IV.1. *For a Δ-free cyclic graph, a matrix realization $B \geq 0$ exists such that $M(B) \not\geq 0$.*

Using Proposition IV.1, we present a simple protocol to construct families of PPT entangled Δ-free "graph" states in arbitrary $d_1 \otimes d_2$ dimensions ($d_1, d_2 \geq 4$):

Step 1. Choose a Δ-free cyclic graph G on d vertices.

Step 2. Construct a matrix realization $B \in \mathcal{M}_d$ of G such that $B \geq 0$ and $M(B) \not\geq 0$.

Step 3. Construct a family F_B of matrix pairs (A, C) in the following manner: choose $A \succcurlyeq 0$, $C \geq 0$ such that $G(A) = G(B) = G(C) = G$, $\operatorname{diag} A = \operatorname{diag} B = \operatorname{diag} C$ and $A_{ij}A_{ji} \geq \max\{|B_{ij}|^2, |C_{ij}|^2\}\ \forall i,j$. (Impose the extra constraint $\sum_{i,j} A_{ij} = 1$ to ensure trace normalization). Then, the two matrix-parameter ($\sim d^2$ real parameters) family $\{\rho_{A,B,C}\}_{(A,C)\in F_B}$ represents a class of $d \otimes d$ G-PPT entangled LDOI states, associated with the Δ-free cyclic graph G and its matrix realization $B \geq 0$ such that $M(B) \not\geq 0$. Exploiting the concluding discussion from Section III, the construction can be easily generalized to arbitrary dimensions with $d_1 \neq d_2$.

We use the above method to explicitly construct a C_4-PPT entangled family of LDOI states in Appendix B. Let us pause here for a moment to appreciate the richness of the above construction. There is an immense variety of Δ-free (cyclic) graphs, which directly translates into a similar variety in the realm of PPT entangled graph states. To gain perspective, we list the number of distinct (connected) Δ-free cyclic graphs on $d \geq 4$ unlabelled vertices in the following sequence (obtained by subtracting the sequences [29, A024607 − A000055]):

$$1, 3, 13, 48, 244, 1333, 9726, 90607, 1143510 \ldots \quad (7)$$

For instance, in a $15 \otimes 15$ system, the $\sim 10^{10}$ (connected) Δ-free cyclic graphs correspond to $\sim 10^{10}$ distinct classes of PPT entangled graph states. Within each class, the $\sim 15^2$ real parameters and different matrix realizations B of the respective graphs further increase diversity.

V. GOING BEYOND Δ-FREE STATES

Let $\rho \in \mathcal{M}_d \otimes \mathcal{M}_d$ be such that the associated matrix A has a triangle containing graph $G(A)$, which means that the test in Theorem III.4 is inapplicable. Nevertheless, there may exist induced subgraphs $\widetilde{G}$ within $G(A)$ [these are of the form $G(\widetilde{A})$ for $\widetilde{d} \times \widetilde{d}$ principal submatrices $\widetilde{A}$ of A, $\widetilde{d} < d$] which are Δ-free. For such a $\widetilde{G}$, let us define the projector $P = \sum_i |i\rangle\langle i|$, where the sum runs over those rows/columns $i \in [d]$ which are present in $\widetilde{A}$. Clearly, $(P \otimes P)\rho(P \otimes P)$ is then Δ-free and hence a valid candidate for Theorem III.4. Using this technique, we have been able to successfully detect entanglement in several randomly generated $d \otimes d$ non Δ-free LDOI states (where $d \sim 20$), see Appendix C for a toy example. Note, however, that the complexity of this method scales badly with d, since the problem of determining the existence of Δ-free induced subgraph in a graph can be easily linked to the problem of finding independent sets in a graph, which is known to be NP-complete [30].

VI. CONCLUSION

In this letter, we have presented a simple test to detect a new kind of bipartite entanglement, which is present in states with a peculiar Δ-free distribution of zeros on their diagonals. From our recipe to construct families of PPT entangled Δ-free states in arbitrary dimensions, it is evident that the ease of Δ-free entanglement detection does in no way restrict its diversity. We have also established an intriguing link between the problems of detecting entanglement in non Δ-free states and finding Δ-free induced subgraphs within a given graph. Several avenues of research stem from our work. The most obvious question to ask is whether the usual entanglement criteria – such as the realignment [31, 32] or the covariance [33] criterion – can detect entanglement in Δ-free states? In a more practical setting (especially when the full state-tomography is impossible [34]), one would like to know the structure of the entanglement witnesses, which can detect this kind of entanglement. These questions are not straightforward to answer because of the incredibly diverse nature of Δ-free entanglement. For example, even if we consider the most trivial family of C_4-PPT entangled Δ-free states from Appendix B, the 18 real parameters inside provide the states with ample freedom to evade detection from any of the usual entanglement tests. We have even been able to tweak the parameters so that the semi-definite hierarchies from [15, 16] give up on detecting entanglement in any reasonable time-frame. Hence, one can deduce that our comparison matrix entanglement test is highly non-trivial and has strong potential to provide drastic computational speed-ups over its regular counterparts in a variety of circumstances. We now conclude our discussion with a few pertinent remarks.

Firstly, an incisive reader might have already noted that the property of Δ-freeness of a state is basis-dependent. In other words, if $\rho \in \mathcal{M}_d \otimes \mathcal{M}_d$ is Δ-free and $U, V \in \mathcal{M}_d$ are unitary matrices, then $(U \otimes V)\rho(U \otimes V)^\dagger$ need not be Δ-free. Thus, a natural question arises: Is there a basis-independent description of the Δ-free property of a state? More specifically, given $\rho \in \mathcal{M}_d \otimes \mathcal{M}_d$, how does one guarantee the existence of local unitaries $U, V \in \mathcal{M}_d$ such that $(U \otimes V)\rho(U \otimes V)^\dagger$ is Δ-free? The answer to the above question can give us insights into what it physically means for a state to be Δ-free. Other entanglement-theoretic properties of Δ-free states (distillability, entanglement cost, etc.) deserve further scrutiny.

Secondly, observe that our main result relies heavily on Theorem III.2, where the idea is to show that the vectors $\{|v_k\rangle, |w_k\rangle\}_{k\in I}$ in the TCP decomposition of (A, B, C) have small common support ($\sigma(v_k \odot w_k) \leq 2$ for each k). While the Δ-freeness of $\rho_{A,B,C}$ is sufficient to guarantee this, it is clearly not necessary. Thus, other constraints on $\rho_{A,B,C}$ which ensure that the above property holds can allow one to detect analogues of Δ-free entanglement. More generally, a hierarchy of constraints $\sigma(v_k \odot w_k) \leq n$ for $n \in \mathbb{N}$ on vectors $\{|v_k\rangle, |w_k\rangle\}_{k\in I}$ in the TCP decompositions of (A, B, C) can be analysed to see if they entail simple necessary conditions on separability of $\rho_{A,B,C}$. Sizeable work along these directions is currently in progress [35].

Acknowledgements. I would like to thank Ion Nechita for helpful insights and stimulating discussions on this topic. This work is partially supported by an INSPIRE Scholarship for Higher Education by the Department of Science and Technology, Government of India.

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Appendix A: Proofs

Proof of Proposition III.5. Observe that $M(B) \geq 0$ if and only if $\det M(\widetilde{B})$ is non-negative for all principal submatrices $\widetilde{B}$ of B (which also correspond to acyclic graphs $G(\widetilde{B})$ if $G(B)$ is acyclic). Hence, to prove the result, it suffices to show that $\det M(B)$ is non-negative for an arbitrary $B \geq 0$ such that $G(B) = (V, E)$ is acyclic. With this end in sight, we first recall the formula:

$$\det B = \sum_{\sigma \in S_d} B_\sigma = \sum_{\sigma \in S_d} (-1)^\sigma \prod_{i\in[d]} B(i, \sigma_i)$$

where the summation occurs over all permutations σ with -1^σ denoting their signs. Now, for some $B_\sigma \neq 0$, we claim that if $\{i, j\} \in E$ is an edge for $i \neq j = \sigma_i$, then $\sigma_j = i$, which implies that B_σ contains a factor of $|B_{ij}|^2$. Since this factor stays invariant as B becomes $M(B)$, the preceeding claim implies that $\det M(B) = \det B \geq 0$, which is precisely our requirement. We now prove the claim. Assume on the contrary that $\sigma_j = k \notin \{i, j\}$. Then, since $B_\sigma \neq 0$, $B(j, k) \neq 0 \implies \{j, k\} \in E$. Now, if $\sigma_k = i$, then $\{i, j\}, \{j, k\}, \{k, i\}$ forms a triangle, which contradicts the fact that $G(B)$ is acyclic. Hence $\sigma_k = l \notin \{i, j, k\}$ and, as before, $\{k, l\} \in E$. Continuing in the fashion, it becomes evident that the sequence of edges $\{i, j\}, \{j, k\}, \{k, l\}, \ldots$ must eventually terminate in a cycle, which is not possible since G is acyclic. $\square$

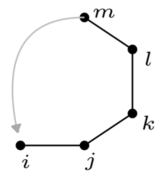


Figure 1: The sequence of edges $\{\{i,j\},\{j,k\},\{k,l\},\dots\} \subset E$ in the proof of Proposition III.5 eventually terminates in a cycle.

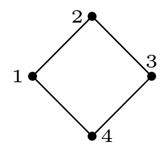
Proof of Proposition IV.1. We first show that the result holds for k-cycles. Assume $k = 4$. Let $B = XX^T$, where

$$X = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & -1 & 0 \end{pmatrix} \quad B = \begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & -1 \\ 1 & 0 & -1 & 2 \end{pmatrix} \tag{A1}$$

Clearly, $B \geq 0$, $G(B) = C_4$ and $M(B) \ngeq 0$. Similar construction can be employed for arbitrary $k > 4$, by defining X as a $k \times (k-1)$ matrix entrywise: $X_{ii} = 1$ for $i \in [k-1]$, $X_{i+1,i} = 1$ and $X_{ki} = (-1)^{i+1}$ for $i \in [k-2]$, and $B = XX^T$. It is then easy to see see that $B \geq 0$, $G(B) = C_4$ and $M(B) \ngeq 0$. Now, let G be an arbitrary Δ-free graph on d vertices with $C_k \subseteq G$. Let $B' \in \mathcal{M}_d$ be such that it contains the above constructed B as the principal submatrix corresponding to the vertices which form the cycle C_k, with all other entries defined to be zero. Let the adjacency matrix of G be $\operatorname{ad} G$. Then, it is easy to see that for every $x > 0$, $\exists\, 0 \neq y \in \mathbb{C}$ with $|y| \leq x$ such that $xI_d + y \operatorname{ad} G \geq 0$. Now, observe that $B_x = B' + xI_d + y \operatorname{ad} G \geq 0$ for all $x > 0$, and $B' = \lim_{x\to 0^+} B_x$ is such that $M(B') \ngeq 0$. Since the cone of positive semi-definite matrices is closed in $\mathcal{M}_d$, we can deduce that there exists an $x > 0$ such that $B = B_x \geq 0$, $M(B) \ngeq 0$ and $G(B) = G$, thus finishing the proof. $\square$

Appendix B: C_4-PPT entangled LDOI family

In this appendix, we use the protocol from Section IV to construct a family of PPT entangled Δ-free graph states in $\mathcal{M}_4 \otimes \mathcal{M}_4$. We begin by choosing the unique Δ-free (connected) graph on 4 vertices: the 4-cycle C_4. Next, we take the matrix realization $B \geq 0$ ($M(B) \ngeq 0$) of C_4 from Eq. (A1). We now construct the family F_B of matrix pairs (A, C) as follows. Firstly, observe from the general form of A, C given in Eq. (B1) that A, B, C have equal diagonals and $G(A) = G(B) = G(C) = C_4$. Notice that even though a_{13} may be non-zero, $G(A)$ doesn't contain the edge $\{1,3\}$ as $a_{31} = 0$. Moreover, it is easy to choose complex numbers c_{ij} such that $C \geq 0$. For this illustration, we simply impose the constraint that $c_{ii} \geq \sum_{j\neq i} |c_{ij}|$ for each $i \in [4]$, so that C becomes diagonally dominant and hence positive semi-definite. Finally, let a_{ij} be non-negative real numbers such that $a_{ij}a_{ji} \geq \max\{|b_{ij}|^2, |c_{ij}|^2\}\, \forall i,j \in [4]$. With these constraints in place, we obtain our family of C_4-PPT entangled states with ~ 18 real parameters: $\{\rho_{A,B,C} \in \mathcal{M}_4 \otimes \mathcal{M}_4 : (A,C) \in F_B\}$. To impose trace normalization, use the fact that $\operatorname{Tr} \rho_{A,B,C} = \sum_{i,j} A_{ij}$.

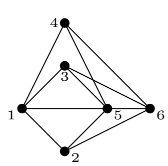
$G(A) =$ 

$$A = \begin{pmatrix} 1 & a_{12} & a_{13} & a_{14} \\ a_{21} & 2 & a_{23} & 0 \\ 0 & a_{32} & 2 & a_{34} \\ a_{41} & a_{42} & a_{43} & 2 \end{pmatrix} \tag{B1}$$

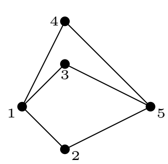
$$B = \begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & -1 \\ 1 & 0 & -1 & 2 \end{pmatrix} \quad C = \begin{pmatrix} 1 & c_{12} & 0 & c_{14} \\ \overline{c_{12}} & 2 & c_{23} & 0 \\ 0 & \overline{c_{23}} & 2 & c_{34} \\ \overline{c_{14}} & 0 & \overline{c_{34}} & 2 \end{pmatrix}$$

Appendix C: Entanglement detection in non Δ-free states

Consider an un-normalized $6 \otimes 6$ PPT CLDUI state $\rho_{A,B}$ with matrices $A, B \in \mathcal{M}_6$ defined in Eq. (C1). Clearly, Theorem III.4 is not applicable here, since $G(A)$ contains a lot of triangles. However, just by removing the 5$^{\text{th}}$ row and column from A, we obtain the principal submatrix $\widetilde{A}$ with a nice Δ-free graph $G(\widetilde{A})$. Moreover, since $M(\widetilde{B}) \ngeq 0$, Theorem III.4 tells us that $\rho_{A,B}$ is entangled.

$G(A) =$ 

$$A = \begin{pmatrix} 11 & 9 & 6 & 6 & 4 & 0 \\ 10 & 13 & 4 & 1 & 11 & 8 \\ 5 & 0 & 13 & 4 & 7 & 8 \\ 6 & 0 & 0 & 13 & 11 & 12 \\ 2 & 9 & 5 & 14 & 15 & 14 \\ 4 & 10 & 4 & 10 & 14 & 11 \end{pmatrix} \quad B = \begin{pmatrix} 11 & -7 & 1 & -3 & -1 & 0 \\ -7 & 13 & 0 & 0 & 6 & 7 \\ 1 & 0 & 13 & 0 & -2 & 3 \\ -3 & 0 & 0 & 13 & -9 & -8 \\ -1 & 6 & -2 & -9 & 15 & 10 \\ 0 & 7 & 3 & -8 & 10 & 11 \end{pmatrix} \tag{C1}$$

$G(\widetilde{A}) =$ 

$$\widetilde{A} = \begin{pmatrix} 11 & 9 & 6 & 6 & 0 \\ 10 & 13 & 4 & 1 & 8 \\ 5 & 0 & 13 & 4 & 8 \\ 6 & 0 & 0 & 13 & 12 \\ 4 & 10 & 4 & 10 & 11 \end{pmatrix} \quad \widetilde{B} = \begin{pmatrix} 11 & -7 & 1 & -3 & 0 \\ -7 & 13 & 0 & 0 & 7 \\ 1 & 0 & 13 & 0 & 3 \\ -3 & 0 & 0 & 13 & -8 \\ 0 & 7 & 3 & -8 & 11 \end{pmatrix} \tag{C2}$$